

⑤ Radial Equation : $V(\vec{r}) = V(r)$

$$-\frac{\hbar^2}{2m} \left[\frac{\partial^2}{\partial r^2} + \frac{2}{r} \frac{\partial}{\partial r} + V_{\text{eff}}^{(l)}(r) \right] R_{nl}(r) = E R_{nl}(r)$$

$$\downarrow R \equiv \frac{u(r)}{r}$$

$$\parallel V_{\text{eff}}^{(l)}(r) = V(r) + \frac{l(l+1)}{2mr^2} \hbar^2$$

... an effective potential.

$$-\frac{\hbar^2}{2m} \frac{d^2 u}{dr^2} + V_{\text{eff}}^{(l)}(r) u(r) = E u(r)$$

1D Schrödinger eq.

* normalization

• Behavior at $r \rightarrow 0$.

$$1 = \int r^2 dr |R|^2 = \int dr r^2 |u|^2$$

We may write $u(r) \sim r^s$ at $r \rightarrow 0$ if it well-behaves.

$$\Rightarrow -\frac{\hbar^2}{2m} s(s-1) r^{s-2} + V(r) r^s + \frac{l(l+1)}{2m} \hbar^2 r^{s-2} = E r^s$$

Leading-order terms

\parallel assume that $r^2 V(r) \rightarrow 0$ as $r \rightarrow 0$.

$$\Rightarrow s(s-1) = l(l+1)$$

$$\therefore s = l+1 \quad \text{or}$$

$$s = -l$$

unphysical!



$$R_{nl}(r) \sim r^l \text{ as } r \rightarrow 0.$$

★ The wave fn. vanishes at $r=0$ unless $l=0$.

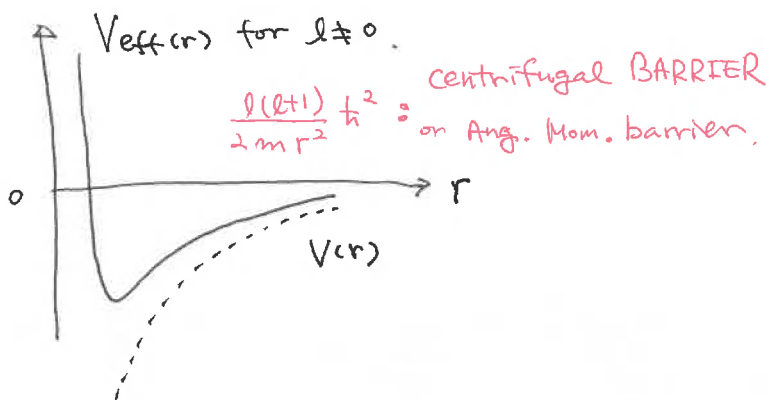
why? Normalization

$$\int_0^\infty dr r^{-2l} : \text{undefined when } l \geq 1$$

$$\text{if } l=0, R \sim \frac{1}{r}$$

$$\Rightarrow \nabla^2 \frac{1}{r} = 4\pi \delta(\vec{r})$$

But the Schrödinger eq has no source!



⑥ Infinite Spherical Well : $V = \begin{cases} 0 & r < a \\ \infty & r > a \end{cases}$

$$-\frac{\hbar^2}{2m} \left(\frac{d^2 R}{dr^2} + \frac{2}{r} \frac{dR}{dr} \right) + \frac{l(l+1)}{2mr^2} \hbar^2 R = E R$$

by setting $k = \sqrt{\frac{2mE}{\hbar^2}}$, and $\rho = kr$

$$\rightarrow \frac{d^2 R}{d\rho^2} + \frac{2}{\rho} \frac{dR}{d\rho} + \left[1 - \frac{l(l+1)}{\rho^2} \right] R = 0$$

Sol. $R(\rho) = \begin{cases} j_l(\rho) = (-\rho)^l \left[\frac{1}{\rho} \frac{d}{d\rho} \right]^l \left(\frac{\sin \rho}{\rho} \right) : \text{spherical Bessel fn.} \\ n_l(\rho) = -(-\rho)^l \left[\frac{1}{\rho} \frac{d}{d\rho} \right]^l \left(\frac{\cos \rho}{\rho} \right) : \text{spherical Neumann fn.} \end{cases}$

But, $n_l(\rho) \rightarrow \rho^{-l-1}$ as $\rho \rightarrow 0$.

$\therefore R(\rho) \propto j_l(\rho)$: unphysical!
 $\rightarrow \sim \rho^l$ as we argued it has to be.

boundary condition

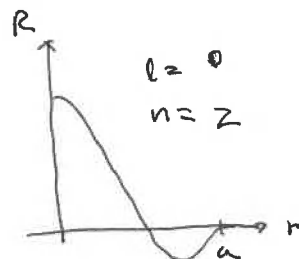
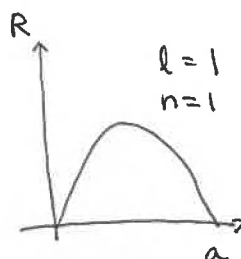
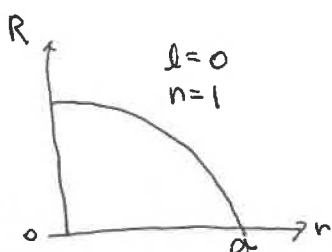
$j_l(ka) = 0 \rightarrow \text{quantization of } E$

ex. $l=0$: $j_0(ka) = \frac{\sin ka}{ka} = 0$

$\rightarrow ka = n\pi$

$E_{l=0} = \frac{\hbar^2}{2m} \left(\frac{n\pi}{a} \right)^2 \quad \parallel \quad n = 1, 2, 3, \dots$

ex. $l=1$: $j_1(ka) = \frac{\sin ka}{(ka)^2} - \frac{\cos ka}{ka}$: needs numerics. to compute $E_{l=1}$.



⑦ The Hydrogen Atom.

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$$V(\vec{r}) = -\frac{Ze^2}{r}$$

one-body problem.

r : relative coordinate.

$m = \mu$: reduced mass

$$= \frac{m_e m_p}{m_e + m_p} \approx m_e \quad (m_p \gg m_e)$$



Two-body problem.

$$\Rightarrow \text{radial equation: } \left[-\frac{\hbar^2}{2m} \frac{d^2}{dr^2} + \frac{l(l+1)\hbar^2}{2mr^2} - \frac{Ze^2}{r} \right] u = Eu$$

by setting $\rho \equiv kr$ where $k = \sqrt{\frac{2m|E|}{\hbar^2}}$ $\parallel E < 0$.

$$\Rightarrow \frac{d^2 u}{d\rho^2} - \frac{l(l+1)}{\rho^2} u + \left(\frac{\rho_0}{\rho} - 1 \right) u = 0$$

$$\text{where } \rho_0 = \sqrt{\frac{2m}{|E|}} \cdot \frac{Ze^2}{\hbar} = \sqrt{\frac{2mc^2}{|E|}} \cdot Z\alpha$$

($\alpha \equiv \frac{e^2}{\hbar c} \approx 1/137$: fine structure const.)

In the limit of $\rho \rightarrow \infty$,

$$\frac{d^2 u}{d\rho^2} - u = 0 \rightarrow u \sim \begin{cases} e^{-\rho} \\ e^{\rho} \end{cases} \quad \text{unphysical.}$$

So, we can attempt to find a solution in the form of

$$u(\rho) = \rho^{l+1} e^{-\rho} w(\rho)$$

$$\Rightarrow \rho \frac{d^2 w}{d\rho^2} + 2(l+1-\rho) \frac{dw}{d\rho} + [\rho_0 - 2(l+1)] w(\rho) = 0$$

Try a power-series solution

$$w(\rho) = \sum_{k=0}^{\infty} c_k \rho^k \quad \parallel c_0 \neq 0!$$

to keep the behavior at $r \rightarrow \infty$.

$$\rightarrow \sum_{k=2}^{\infty} C_k \cdot k \cdot (k-1) e^{k-1} + 2(l+1) \sum_{k=1}^{\infty} C_k \cdot k \cdot e^{k-1}$$

$$- 2 \sum_{k=1}^{\infty} C_k \cdot k \cdot e^k + [p_0 - 2(l+1)] \sum_{k=0}^{\infty} C_k e^k = 0$$

$$\rightarrow \sum_{k=1 \rightarrow 0}^{\infty} C_{k+1} (k+1) \cdot k e^k + \sum_{k=0}^{\infty} (2l+2) C_{k+1} (k+1) e^k$$

$$+ \sum_{k=1 \rightarrow 0}^{\infty} (-2) C_k \cdot k \cdot e^k + [p_0 - 2(l+1)] \sum_{k=0}^{\infty} C_k e^k = 0$$

$$\rightarrow \sum_{k=0}^{\infty} \left[[k(k+1) + 2(l+1)(k+1)] C_{k+1} - [2k + 2(l+1) - p_0] C_k \right] e^k = 0$$

$$\therefore \frac{C_{k+1}}{C_k} = \frac{2k + 2l + 2 - p_0}{(k+1)(k+2l+2)} \sim \frac{2}{k} \text{ as } k \rightarrow \infty$$

if p_0 is not an integer
positive.

: This is a problem.

because $\frac{C_{k+1}}{C_k} \sim O\left(\frac{1}{k}\right)$ gives $W(r) \sim \exp[5r]$,
and then it changes the asymptotic behavior.

\Rightarrow Therefore, the term C_k has to be terminated
at some power $k=N$, s. t.

$$\therefore p_0 = \boxed{\text{positive integer}} = 2(N+l+1) \equiv 2n$$

$$\Rightarrow E = - \frac{1}{2} mc^2 (Z\alpha)^2 \cdot \frac{1}{n^2} \quad \parallel \quad n = \overbrace{N+l+1}^{0,1,2,\dots} = 1, 2, 3, 4, \dots$$

$\underbrace{13.6 \text{ eV} \cdot Z^2}$

\rightarrow $n=1 \dots l=0$ only allowed.
"principal quantum number"
 $n=2 \dots l=0, 1$
 $n=3 \dots l=0, 1, 2$
 \vdots

degeneracy of $E_n \leftarrow \# \text{ of } |n, l, m\rangle \text{ for a given } n.$ 49

$$= \sum_{l=0}^{n-1} 2l+1 = \underline{n^2}$$

• The length scale κ in $\rho = \kappa r$ also n -dependent!

$$\frac{1}{\kappa} = \frac{\hbar}{m c \alpha} \frac{n}{Z} \equiv a_0 \frac{n}{Z}$$

\rightarrow natural length scale $a_0 \equiv \frac{\hbar^2}{m c \alpha} = \frac{\hbar^2}{m e^2}$: Bohr radius

• finally, the wave function:

$$\psi_{n\ell m}(\vec{x}) = R_{n\ell}(r) Y_{\ell}^m(\theta, \phi).$$

$$R_{n\ell}(r) = \left(\frac{Z}{na_0}\right)^l \cdot e^{-\frac{Zr}{na_0}} \sum_{k=0}^{\infty} C_k \left(\frac{Z}{na_0} r\right)^k$$

$$\text{where } \frac{C_{k+1}}{C_k} = \frac{2(k+l+1-n)}{(k+1)(k+2l+2)}.$$

• C_0 has to be determined by the normalization

$$\int_0^{\infty} r^2 dr |R_{n\ell}|^2 = 1.$$

• The other example in the S & N is
the isotropic simple Harmonic Oscillator.

\leftarrow Try to solve it by yourself.

Caution: the asymptotic behavior at a large r
is different.

* Implications of the degeneracy " n^2 ": Is it accidental? 50

(S&N. ch.4.1)

for a given n , $l = 0, 1, \dots, n-1$ are allowed.

→ Maybe there exists some symmetry higher than $SO(3)$.

[$SO(3)$ indicates only $m = -l \dots l$ for a given l .]

• In the Kepler problem in C.M. ($F(\vec{r}) = -\frac{k}{r^2} \hat{r}$)

$\vec{A} = \vec{p} \times \vec{L} - m k \hat{r}$ is conserved.

: Laplace-Runge-Lenz or Runge-Lenz or Lenz vector.

→ The perihelion does not change in time.

• In Q.M., a Hermitian version of the Lenz vector:

$$\vec{M} = \frac{1}{2m} (\vec{p} \times \vec{L} - \vec{L} \times \vec{p}) - \frac{Ze^2}{r} \vec{x}$$

For two Hermitian \vec{A}, \vec{B} ,

$$(\vec{A} \times \vec{B})^+ = -\vec{B} \times \vec{A}$$

$$\Rightarrow \underline{[\vec{M}, H] = 0} \quad \text{for } H = \frac{\vec{p}^2}{2m} - \frac{Ze^2}{r}$$

one can also find

$$\vec{L} \cdot \vec{M} = \vec{M} \cdot \vec{L} = 0$$

$$\vec{M}^2 = \frac{Ze^2}{m} H (\vec{L}^2 + \hbar^2) + Ze^4$$

and

$$[L_i, L_j] = i\hbar \epsilon_{ijk} L_k$$

$$[M_i, M_j] = -i\hbar \epsilon_{ijk} \frac{Ze^2}{m} H L_k$$

$$[M_i, L_j] = i\hbar \epsilon_{ijk} M_k$$

This prevents us to make

a closed algebra,

but, we can make it closed

by considering energy eigenstates.

$$\rightarrow H = E$$

$$[L_i, L_j] = i\hbar \epsilon_{ijk} L_k$$

$$[N_i, N_j] = i\hbar \epsilon_{ijk} L_k$$

$$[N_i, L_j] = i\hbar \epsilon_{ijk} N_k$$

$$\Leftrightarrow \vec{N} = \left(-\frac{m}{2E}\right)^{\frac{1}{2}} \vec{M}$$

★ 6 generators of $SO(4)$; rotations in 4D.

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But, we can separate the algebra of $SO(4)$ into two sets of algebras.

If we define

$$\begin{cases} \vec{I} \equiv (\vec{L} + \vec{N})/2 \\ \vec{K} \equiv (\vec{L} - \vec{N})/2 \end{cases} \quad \parallel \quad \begin{matrix} \text{NOTE:} \\ [\vec{I}, H] = 0 \\ [\vec{K}, H] = 0 \end{matrix}$$

$$\Rightarrow [I_i, I_j] = i\hbar \epsilon_{ijk} I_k, \quad [K_i, K_j] = i\hbar \epsilon_{ijk} K_k, \quad [I_i, K_j] = 0$$

$\downarrow SU(2) \qquad \qquad \qquad \downarrow SU(2)$

$$I^2 \rightarrow \tilde{n}(\tilde{n}+1)\hbar^2 \quad \parallel \tilde{n} = 0, \frac{1}{2}, 1, \frac{3}{2}, \dots \quad (2\tilde{n}+1) \text{ deg.}$$

$$K^2 \rightarrow k(k+1)\hbar^2 \quad \parallel k = 0, \frac{1}{2}, 1, \frac{3}{2}, \dots \quad (2k+1) \text{ deg.}$$

Since $\vec{I}^2 - \vec{K}^2 = \vec{L} \cdot \vec{N} = 0, \quad k = \tilde{n}.$

The operator $\vec{I}^2 + \vec{K}^2 = \frac{1}{2} [\vec{L}^2 - \frac{m}{2E} \vec{M}^2]$

goes to $2k(k+1)\hbar^2 = \frac{1}{2} \left(-\hbar^2 - \frac{m}{2E} Z^2 e^4 \right)$

$$E = - \frac{m Z^2 e^4}{2\hbar^2} \frac{1}{(2k+1)^2}, \quad k = 0, \frac{1}{2}, 1, \frac{3}{2}, \dots$$

$$= - \frac{m Z^2 e^4}{2\hbar^2} \frac{1}{n^2}, \quad n = 1, 2, 3, 4, \dots$$

$\parallel \vec{M}^2 = \frac{2}{m} H (\vec{L}^2 + \hbar^2) + Z^2 e^4.$

$\therefore \text{deg.} = (2\tilde{n}+1) \cdot (2k+1) \big|_{k=\tilde{n}} \text{ for a given } n.$

$= n^2$

$SO(4) = SU(2) \times SU(2)$